Inverse design of nonlinear mechanical metamaterials via video denoising diffusion models

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Abstract

The accelerated inverse design of complex material properties—such as identifying a material with a given stress–strain response over a nonlinear deformation path—holds great potential for addressing challenges from soft robotics to biomedical implants and impact mitigation. Although machine learning models have provided such inverse mappings, they are typically restricted to linear target properties such as stiffness. Here, to tailor the nonlinear response, we show that video diffusion generative models trained on full-field data of periodic stochastic cellular structures can successfully predict and tune their nonlinear deformation and stress response under compression in the large-strain regime, including buckling and contact. Key to success is to break from the common strategy of directly learning a map from property to design and to extend the framework to intrinsically estimate the expected deformation path and the full-field internal stress distribution, which closely agree with finite element simulations. This work thus has the potential to simplify and accelerate the identification of materials with complex target performance. Machine learning models have been widely used in the inverse design of new materials, but typically only linear properties could be targeted. Bastek and Kochmann show that video diffusion generative models can produce the nonlinear deformation and stress response of cellular materials under large-scale compression.